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Theoretical Study of Electron Mobility in Modulation-Doped Aluminum Gallium Arsenide

Gallium Arsenide

Benjamin Segall
*Lewis Research Center
Cleveland, Ohio*



National Aeronautics
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Summary

The high electron mobilities observed in modulation-doped aluminum gallium arsenide—gallium arsenide (AlGaAs—GaAs) layered heterostructures make these structures interesting for potential microwave and high-speed logic applications. A theoretical study of the mobility at moderately high temperatures, $T \gtrsim 100$ K, is undertaken. It is suggested that, as usual, the dominant scattering mechanism limiting the mobility in the temperature range of interest is that involving the absorption of longitudinal optical (LO) phonons. It is further suggested that the screening of this polar mode scattering by the relatively high carrier concentration in the channel leads to a significant increase in the mobility. The contributions of scattering from ionized (unintentional) impurities in the channel and from the asperities on the interface are also taken into account. It is found that the resultant calculated mobilities are in reasonable agreement with the measured values and that the screening of polar mode scattering enhances the mobility by approximately 50 percent. Comparison between the calculated and measured mobilities also suggests that the quantization effects are relevant for temperatures up to about 100 K.

Introduction

Interest in device applications for the semiconductor gallium arsenide (GaAs) has increased sharply as the need for semiconducting components that operate in the microwave region of the electromagnetic spectrum has become apparent. The reason is primarily that GaAs has a considerably higher electron mobility and hence a shorter response time than does silicon. Interest has also grown in layered heterojunction structures involving GaAs such as aluminum gallium arsenide—gallium arsenide (AlGaAs—GaAs) because of their anticipated uses in a variety of devices. Initially, however, such structures had disappointingly low mobilities (ref. 1) which concomitantly would reduce their usefulness at high frequencies. A significant advance in this area was made with the introduction of the modulation doping (ref. 1) technique, which involves doping only the semiconductor component with the larger band gap—for example, the AlGaAs in the AlGaAs—GaAs structure. The resulting structures showed a marked increase in mobility (refs. 2 and 3) with values of the more recent samples being comparable to those found in good bulk GaAs.

The observed behavior was interpreted (ref. 1) by noting that because of the appreciably wider band gap in the AlGaAs the donor impurity (generally silicon) levels in it are at higher energies than the GaAs conduction

band edge. As a result, some of the donated electrons fall into the GaAs conduction band. The schematic in figure 1 depicts the electronic structure around the interface for the case in which the GaAs is weakly n-type. The electrons are confined to a channel along the interface by the electrostatic forces resulting from the charge transfer. The electrostatic forces, of course, produce the band bending. The observed high mobility μ was attributed to the absence of significant ionized impurity scattering in the undoped and hence relatively pure GaAs. The highest mobility samples are those in which there is an undoped region in the AlGaAs of depth d (about 150 Å or so) from the interface (see fig. 1). This insures a reasonable separation of the carriers from their charged donor parents. While the elimination of a high concentration of impurities in the GaAs is certainly an essential factor, it seems that another factor which reduces the scattering must also come into play. The fact that the carriers are confined to a narrow channel with a width of the order of 100 Å, which is a length comparable to the electron mean free path for temperatures around and below 300 K, implies that surface scattering should reduce μ to values below those observed in the bulk. And, there are still other scattering mechanisms (several of which will be discussed) which would further lower μ . To identify the relevant effect that leads to the appreciable increase in μ , which in effect compensates for the previously mentioned reductions, we first note that the principal scattering mechanism for the temperatures of interest in clean bulk semipolar semiconductors involves the interaction with the longitudinal optical (LO) phonons (ref. 4), the so-called polar mode scattering. We also note that the electron concentration in the channels is fairly high. Therefore, we suggest that there may be sufficiently effective electronic screening of the polar mode interaction, whose strength derives principally from its long range character, to lead to the required increase.

In large measure, the purpose of the work described in this report is to verify the previous suggestion. In addition, estimates are made of the contributions of surface scattering and ionized impurity scattering. In this report the temperature range of primary concern is that in which the polar mode scattering is dominant—namely, $T \gtrsim 100$ K. These temperatures, of course, include those in which most practical applications are realized. The upper end of the range is 300 K, since data are not available for temperatures above that value.

An accurate calculation of the mobility in the present problem would be very complex. In addition, there are several parameters in the problem (e.g., the residual impurity and carrier concentrations in the GaAs) which are not presently known accurately. Thus, of necessity, a number of approximations and estimates of parameters must be made. While it seems most useful to discuss these at the appropriate place in the text, the most important of

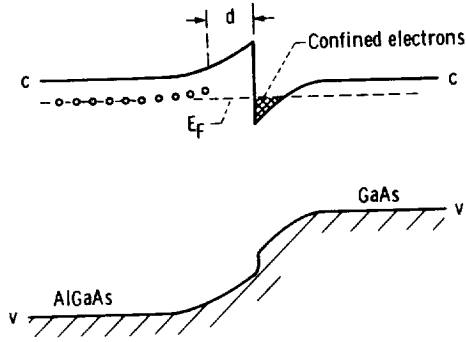


Figure 1. - Schematic energy diagram of a modulation n-doped AlGaAs - GaAs interface with the GaAs weakly n-type. Fermi level, E_F ; conduction band edge, c ; valence band edge, v ; depth in AlGaAs from the interface which is undoped, d .

these approximations is considered here. Because of the confinement of the electrons close to the interface, the motion of the electrons in the direction normal to the interfacial plane is quantized (ref. 5); that is, the electronic spectrum consists of separated (but overlapping) bands corresponding to free electronlike behavior (albeit with the appropriate effective mass) in the two dimensions parallel to the interface. To the extent that only one band, or at most a very small number of bands, is involved, the problem is essentially two-dimensional. Clearly, this is the case at low temperatures—that is, for $T < \Delta E/k_B$ where ΔE is the separation between the lowest energy levels and k_B is Boltzmann's constant. At higher T , the uniquely two-dimensional effects cease to be important and can safely be neglected. We feel that this is the case for temperatures well above 100 K, and we use this assumption in the present work. As a result of this assumption, it is possible to use the results previously developed for the bulk. However, Delagebeaudeuf and Linh (ref. 6) have suggested that the two-dimensional effects are not negligible over a somewhat larger T range than we suggested previously. But we feel that their calculations tend to overestimate the extent of the two-dimensional regime¹. We return to this point in the last section of the report where a comparison is made between the results of the calculations based on our assumption and the data.

Calculations

As noted previously, the dominant mechanism for the T range of interest in clean bulk crystals involves the

¹In dealing with the interface problem, these workers approximate the complete infinite spectrum by two levels. The upper levels then represent the effect of all the excited levels in the channel. The resulting effective level separation must be larger than the true separation between the two lowest levels.

scattering of electrons by the absorption and emission of LO phonons. In the weak coupling approximation, which is appropriate for GaAs (since the relevant parameter $\alpha/6 < 0.01 \ll 1$ where α is the polaron coupling constant, which is defined subsequently), a single phonon is involved. The momentum and energy conservation conditions are then

$$\hbar \vec{k}' = \hbar \vec{k} \pm \hbar \vec{q}$$

and

$$\frac{\hbar^2 k'^2}{2m^*} = \frac{\hbar^2 k^2}{2m^*} \pm \hbar \omega(\vec{q})$$

where \vec{k} and \vec{k}' are the initial and final wave vectors of the electron, \vec{q} the wave vector of the phonon, $\omega(\vec{q})$ its angular frequency (which we take to be relatively constant, i.e., $\omega(\vec{q}) = \omega$), and m^* the effective mass of the electron. The upper and lower signs relate to phonon absorption and emission, respectively. Because of energy conservation the emission process plays no role for T below the characteristic temperature of the LO phonon, namely, $\Theta = \hbar \omega/k_B = 419$ K (ref. 7, p. 72). The scattering rate must then be proportional to, and μ inversely proportional to, the Bose-Einstein occupation factor $[\exp(\Theta/T) - 1]^{-1}$ for the LO phonon.

The solution to the conductivity problem in the presence of (unscreened) polar mode scattering, which is complicated by the fact that one cannot use the relaxation time approximation, was found by Howarth and Sondheimer (ref. 8) in terms of a series of ratios of determinants of increasing size. From their result the following expression for μ_{LO} can be obtained:

$$\mu_{LO} = \frac{0.769}{\alpha \hbar \omega} \left(\frac{m}{m^*} \right)^{1/2} G(z) e^{-\xi} \quad \text{cm}^2/\text{V-sec} \quad (1)$$

with

$$\alpha = \left(\frac{m^*}{m} \right)^{1/2} \left(\frac{13.6}{\hbar \omega} \right)^{1/2} (\epsilon_\infty^{-1} - \epsilon_s^{-1})$$

where $\hbar \omega$ in the previous formulas is given in electron volts, $z = \hbar \omega/k_B T = \Theta/T$, and $G(z) e^{-\xi}$ is an algebraic function of certain Bessel functions $K_n(z/2)$. The previous expressions represent a modification of Howarth and Sondheimer's results in that the electronic charge in their expression is replaced by the appropriate effective charge that should appear in the polar mode coupling (ref. 4).

We have evaluated the expression in equation (1) for GaAs for $100 \text{ K} \lesssim T \lesssim 300 \text{ K}$ using the measured values for m^*/m , $\hbar \omega$, ϵ_s , and ϵ_∞ which are, respectively, 0.068 (ref. 9), 0.0361 eV (ref. 7), 12.9 (ref. 7), and 10.9 (ref. 7).

There are no unknown parameters involved in calculating the unscreened μ_{LO} . The result is shown as the dashed curve in figure 2. For comparison purposes, we show as points the highest reported mobility values for the AlGaAs—GaAs heterostructure which were measured by Drummond et al. (ref. 2). Comparable mobilities were also found by Stormer et al. (ref. 3). As can be seen, the calculated μ_{LO} for the unscreened polar mode scattering agrees fairly well with the data except at low temperatures, but this is certainly not the full story for the reasons alluded to previously. Note that equation (1) is the drift mobility μ_D while the measured values are Hall mobilities μ_H . We will neglect the differences between these since we expect the so-called Hall factor $r = \mu_H / \mu_D$ to be only slightly greater than 1 over the temperature range of interest and for the carrier concentration appropriate to our problem. For bulk GaAs, $r \approx 1.15$ for the relevant temperature range (ref. 7, fig. 12.8, p. 378). In fact, we expect the ratio to be lower than this value since the electron distribution in the channel is more

“degenerate” than in typical bulk material and $r \approx 1.0$ for a degenerate distribution.

The first effect studied was the screening of the lattice polarization by the carriers. This correction has been worked out by Ehrenreich (ref. 10) who obtained a result for μ_{LO} with screening of the same form as equation (1) but in which the factor $G(z)e^{-\xi}$ is replaced by a different function $G(\omega_p, z)e^{-\xi}$. The latter factor is a function of the plasma frequency ω_p , which is given by

$$\omega_p^2 = \frac{4\pi e^2 n}{\epsilon_\infty m^*}$$

with n being the carrier density. Numerical values for this factor as a function of z were presented for a range of ω_p/ω values in figure 2 of Ehrenreich's paper.

In contrast to the usual bulk measurements, the quantity determined in the studies of the electrical properties of the layered structures is not the carrier

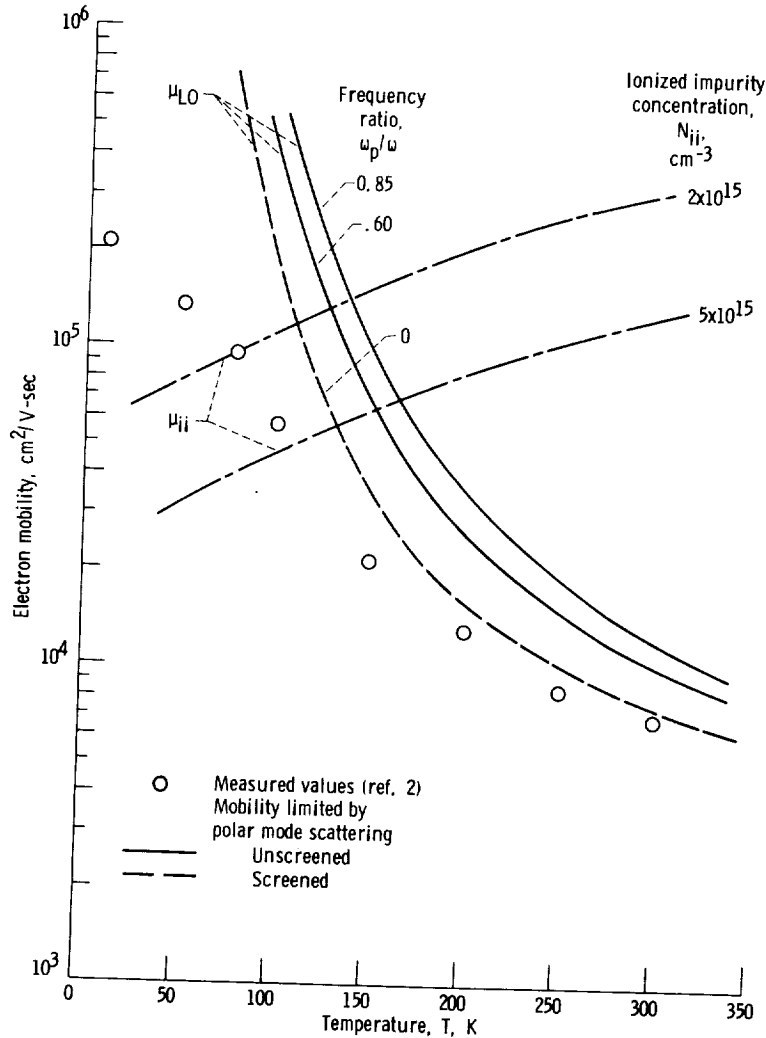


Figure 2. -Electron mobility in GaAs channel of modulation-doped AlGaAs - GaAs heterojunction as function of temperature.

density n but rather the charge per unit area for the particular structure employed. To obtain an estimate of n , it is necessary to know the effective width of the channel. This important parameter is, in fact, not known accurately, but it has been estimated (ref. 5) to be roughly 100 Å at low temperatures ($T \approx 4$ K). Using the measured areal charge density (ref. 2) of 2.5×10^{12} per square centimeter (cm^{-2}), gives a value $n = 5 \times 10^{17} \text{ cm}^{-3}$ and a $\omega_p/\omega = 0.85$ for the particular structure used in the study. At the higher temperatures of interest in this work, it is possible that the effective width will be somewhat larger. For a width twice as large, the density is halved and $\omega_p/\omega = 0.60$. The factor $G(\omega_p, z)e^{-\xi}$ was evaluated for these two ω_p/ω ratios by a suitable interpolation of Ehrenreich's values. From these factors and equation (1) the μ_{LO} 's corresponding to the screened polar mode scattering were calculated. The μ_{LO} 's are shown in figure 2 as two solid curves which lie significantly above the unscreened as well as the measured μ values. These results give a rough estimate of the magnitude of the screening correction and of the uncertainty in our knowledge of it due to the uncertainty in the carrier concentration.

Evidence for the role of other mechanisms is easily seen at $T \gtrsim 100$ K where the data deviate increasingly from the calculated μ resulting from the polar mode scattering which increases exponentially (because of the reciprocal Bose-Einstein factor). In fairly pure bulk semipolar semiconductors such as GaAs, impurity scattering, whose importance increases as T decreases, plays a dominant role at fairly low T , say $T \lesssim 100$ K; this should also be the case for the structures that we are considering even though they are nominally undoped. Unfortunately, there is no reported determination of the impurity concentration in the GaAs. In view of this, we have arbitrarily taken two values for the ionized impurity concentration N_{ii} : $2 \times 10^{15} \text{ cm}^{-3}$ and $5 \times 10^{15} \text{ cm}^{-3}$. These are reasonable values for fairly pure bulk GaAs, and their difference is not an unreasonable indication of the uncertainty in N_{ii} .

A modification of the usual Brooks-Herring formula (ref. 11) has been used to compute the mobility due to the ionized impurity scattering μ_{ii} . In the usual treatment, the concentration of the carriers involved in the screening is related to the impurities producing the scattering. In the present situation that is not the case. In fact, the carrier concentration in the channels is appreciably larger than the impurity concentration assumed previously. The calculated μ_{ii} (which are given as dot-dash curves in fig. 2) rise in the expected manner with increasing T . The impurity scattering becomes ineffective in limiting μ for $T \gtrsim 250$ K.

We now digress to discuss an apparent problem. At $T = 100$ K for the higher value of N_{ii} and $T = 75$ K for the lower value, the μ_{ii} and perforce the μ for the combined scattering mechanisms are lower than the measured

value. The discrepancy is worse at lower T . In part this could be caused by using values of N_{ii} which are too large; however, this does not explain the temperature dependence of the difference. It seems likely that the discrepancy is in large part due to the occurrence of quantization effects, which were mentioned in the Introduction. The quantization and degeneracy effects, both of which become increasingly important at low T , tend to reduce the availability of final states for the scattering and, as a result, the scattering rate.

Returning to the main discussion, we recall that the electrons are confined to a channel having a width comparable to the electron mean free path. As a result, deviations from uniformity of the channel boundaries, particularly on the interface, could significantly affect the mobility. A rigorous treatment of the surface scattering would be more laborious than warranted here. We thus seek a tractable but physically reasonable way to handle this effect. To this end, we note that the configuration of the electrons is similar to that of a film, and therefore, this fact can be used to obtain the needed results. The major difference between the two configurations is that in the film there are effectively abrupt potential jumps at both surfaces while in the heterostructures the confining potential on the GaAs side is relatively gradual. Irregularities on that side are expected to be less effective in scattering than are those on the interface.

Conductivity in a film was treated by Fuchs (ref. 12) in 1938. From his results it is easily shown that the ratio of the mobility in the film μ to that in the bulk μ_0 is given by

$$\frac{\mu(K, p)}{\mu_0} = 1 - \frac{3(1-p)}{2K} \int_1^\infty \left(\frac{1}{t^3} - \frac{1}{t^5} \right) \frac{1 - e^{-Kt}}{1 - pe^{-Kt}} dt \quad (2)$$

where $K = a/l$ with a the film thickness and l the mean free path. The parameter p , the *polish*, gives the fraction of the electrons scattered specularly. Such scattering does not lead to a reduction in the conductivity. For completely diffuse scattering ($p = 0$), which is the situation that is generally taken to prevail at most surfaces, the previous equation reduces to

$$\frac{\mu(K, 0)}{\mu_0} = 1 - \frac{3}{8K} + \frac{3}{2K} [E_3(K) - E_5(K)] \quad (3)$$

where $E_n(x)$ is the exponential integral, which is a tabulated function.

These results are functions of $K = a/l$, and to evaluate them, one must know $l(T)$. Both functions are monotonically increasing functions of K . As indicated earlier, the concept of a mean free path, or relatedly, of a scattering time, is not rigorously valid for the polar mode scattering. We, however, neglect that fine point and take

$$l = (3m^*k_B T)^{1/2} \mu_0 e^{-1} \quad (4)$$

To obtain μ_0 from our estimates of μ_{LO} and μ_{ii} we use Matthiessen's rule, which in the present context is

$$\mu_0^{-1} = \mu_{LO}^{-1} + \mu_{ii}^{-1} \quad (5)$$

and which is generally a good approximation. The l at $T=300$ K, where μ_{LO} is dominant, is about 80 Å and 50 Å for the screened and unscreened polar mode scattering, respectively. At $T=100$ K, l ranges from about 150 Å for $N_{ii}=5 \times 10^{15} \text{ cm}^{-3}$ to about 350 Å for $N_{ii}=2 \times 10^{15} \text{ cm}^{-3}$. In a film having a 100 Å thickness these values of free path indicate that surface roughness will be effective in reducing the mobility with the largest reduction, of course, occurring at the lower temperatures.

We have evaluated equation (3), which gives the surface scattering reduction in the diffuse scattering limit, instead of the more general expression, equation (2), which is valid for all p . This was done because past experience has indicated that surface scattering has generally been quite effective in reducing the conductivity and thereby implying a relatively low value of p . Also, equation (3) can be evaluated more simply than equation (2) because it is given in terms of tabulated functions. The computations were carried out for film thicknesses of 100 and 200 Å. These two values were used to test the sensitivity of the results to film thickness. Also, the calculations were carried out using both the screened and unscreened μ_{LO} in equation (5). The same carrier concentration of $n=5 \times 10^{17} \text{ cm}^{-3}$, corresponding to $\omega_p/\omega=0.85$, was used for the calculations of the screened μ_{LO} for both film thicknesses. The set of mobilities resulting from these computations for an assumed ionized impurity density of $5 \times 10^{15} \text{ cm}^{-3}$ is shown in figure 3(a), while the set for $N_{ii}=2 \times 10^{15} \text{ cm}^{-3}$ is shown in figure 3(b). The measured values of the mobility are shown in both figures as points.

Comparison with Measurements and Conclusions

The results of our study are essentially contained in figures 3(a) and (b). It is seen that the resultant calculated μ 's, which include contributions from the scattering mechanisms that we believe to be dominant and involve reasonable estimates for the parameters characterizing the channel, cluster closely around the measured values over the temperature range of primary interest in this report ($100 \text{ K} \lesssim T \leq 300 \text{ K}$). Moreover, the mobilities obtained using the unscreened LO scattering fall below

the data—except for the curve for $a=200$ Å and $N_{ii}=2 \times 10^{15} \text{ cm}^{-3}$ which almost passes through the data points for $T > 150$ K—while those including the effect of screening lie above the data. In terms of our expectations, this is a satisfactory situation since the contributions to the scattering that were not included (a number of which will be discussed subsequently) would lower the resultant μ somewhat.

The other principal piece of information contained in the figures is the magnitude of the increase in the mobility resulting from the screening of the polar mode scattering. For the two concentrations of ionized impurities and two thicknesses considered, the increase is about 50 percent, a respectable increase. The effect would be larger or smaller if the carrier density is larger or smaller than the value used. With a given areal density, of course, the effective density depends inversely on the width of the channel, which is thus a parameter it is desirable to know more accurately than it is presently known.

A higher carrier concentration would be desirable since it would further increase μ . Possibly an increase could be achieved by heavier doping of the AlGaAs. If this can be accomplished without too great a reduction in channel width,² a further significant increase in mobility would result, and this would be of practical importance.

A mechanism that has not been included and which could possibly affect μ noticeably is the scattering by ionized impurities outside the channel, in particular, those in the AlGaAs which are present in reasonably high density. To obtain an idea about the magnitude of this effect, it is useful to note that in the usual treatment of mobility limited by ionized impurity scattering the scattering involved is from isolated impurities. This is appropriate when the (Debye) screening length is smaller than the interimpurity separation—which is the case in the channel for the parameters assumed in this work. (The former is about 100 Å while the latter is about 1000 Å.) On the other hand, the distance between the carriers and the remote impurities in the AlGaAs is greater than 100 Å, which is roughly the interimpurity distance. (Recall that there is a spacer region between the carriers and the charged donors in the AlGaAs, see fig. 1.) This implies that the carriers do not feel the remote impurities individually. To understand how the remote ionized impurities contribute to the scattering of the free carriers, recall that the field produced from an assumed continuous distribution of the remote impurities leads to the band bending and thus to the formation of the channel in the GaAs. This part of the field thus does not

²It is likely that a heavier doping would lead to a reduction in the channel width a and hence in K . The attendant decrease in $\mu(K, O)/\mu_0$ would then partially offset the increase in μ_0 . The extent of this counteracting effect, which is worthy of further consideration, is presently unknown.

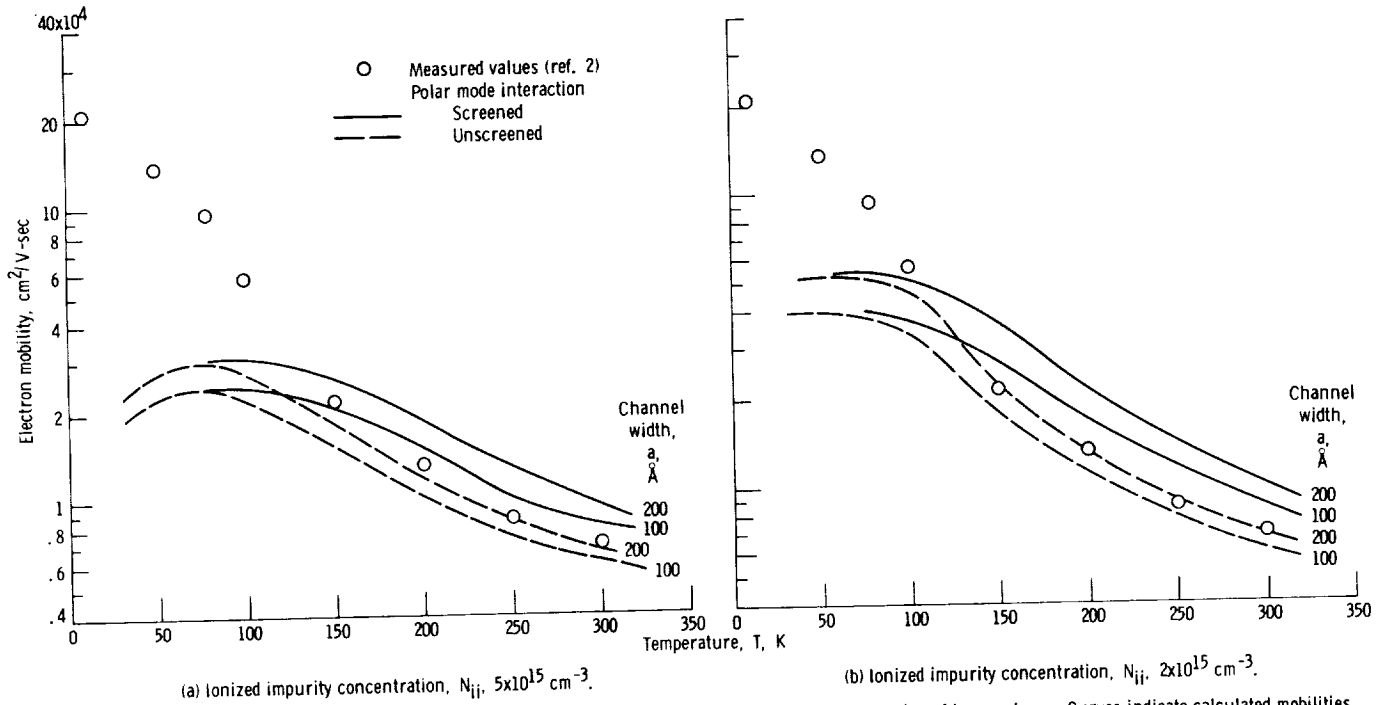


Figure 3. - Electron mobility in GaAs channel of modulation-doped AlGaAs-GaAs heterojunction as function of temperature. Curves indicate calculated mobilities limited by combined effect of polar mode, ionized impurity, and diffuse surface scatterings for channels 100 and 200 Å wide.

contribute to the scattering. The scattering associated with the remote impurities must then result from the fields due to the difference between the actual distribution of the charged donor atoms and the continuous distribution and, consequently, is not expected to be very important. But, we have as yet not estimated this contribution.

Another mechanism that has been neglected in this work is the scattering by the relatively long wave length acoustic phonons; this is generally referred to as scattering by the deformation potential. We have estimated that this contribution will further reduce μ by roughly 5 percent (ref. 13). The estimate was obtained using a published curve of the mobility limited by this scattering mechanism (fig. 7 of ref. 13) and Matthiessen's rule. Yet another mechanism that has not been included is the piezoelectric scattering. This contribution is expected to be quite weak; but again we have not yet estimated its magnitude. Although we do not presently have good estimates for the contributions of the mechanisms that have been neglected in this report, it seems likely they will be small individually but that their inclusion collectively would bring the calculated μ into noticeably better agreement with the data.

The final point concerns our assumption that the effects due to the quantization of the levels in the channel (i.e., the two-dimensionality effects) can be neglected above 100 K or so but not below that temperature. The satisfactory agreement between the various calculated μ 's and the data for $T > 150 \text{ K}$ both in terms of absolute

magnitude and temperature dependence tends to support the assumption. Moreover, it is noteworthy that the discrepancies between the calculated and measured values become appreciable at about $T = 100 \text{ K}$ and, probably more significantly, increase as T decreases. This could be understood in terms of the reduction in final states available for scattering that accompanies the emergence of the two-dimensional behavior; however, degeneracy effects (Fermi statistics) could also play a significant role. Thus, a useful byproduct of this report is some evidence that the crossover between two-dimensional and three-dimensional behavior occurs roughly at 100 K. Admittedly, the evidence is indirect, and the role of degeneracy must be studied. Further investigation is necessary to more accurately pin down the crossover temperature.

Concluding Remarks

The present calculations verify the expectations that scattering by the absorption of LO phonons is the dominant mechanism in determining the electron mobility in modulation n-doped AlGaAs-GaAs heterostructures for temperatures in the range $100 \text{ K} \lesssim T \lesssim 300 \text{ K}$. Furthermore, the screening of the interaction between the carriers and the LO phonons by the fairly high density of electrons in the channels leads to a significant increase in mobility (by about 50 percent) over that expected for the unscreened interaction. It is

suggested that heavier doping of the AlGaAs could lead to a further significant increase in the mobility.

Lewis Research Center
National Aeronautics and Space Administration
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